DIFFRACTION GRATING MONOCHROMATORS (SGMs)

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Advanced Light Source

THE GRATING EQUATION

General reference:
Howells, X-ray Data Booklet, 2001

- Sign convention: α, β have opposite signs if they on opposite sides of the normal
- $m\lambda = d(\sin\alpha + \sin\beta)$
- Given m, λ and d, there are still an infinite number of α, β pairs that satisfy this equation
- Therefore we can impose a relationship between α and β as follows:
- **FIXED IN-OUT DIRECTIONS (SGM):**

$$\alpha - \beta = 2\theta$$

$$m\lambda = 2d\cos\theta\sin(\beta+\theta)$$

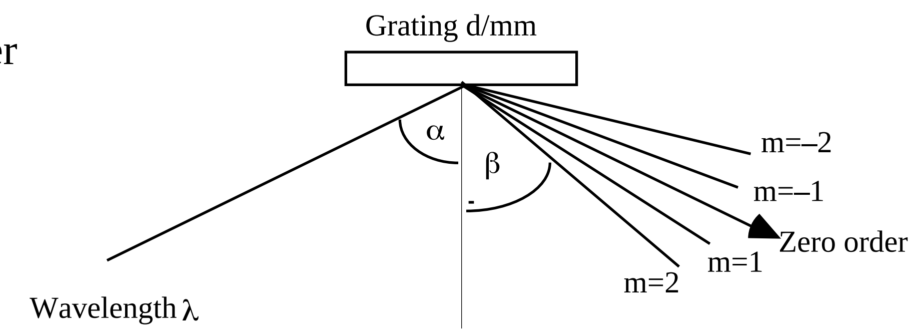
- **In this case there is a "horizon" wavelength:** If α or β becomes 90°, the acceptance falls to zero which happens at wavelength

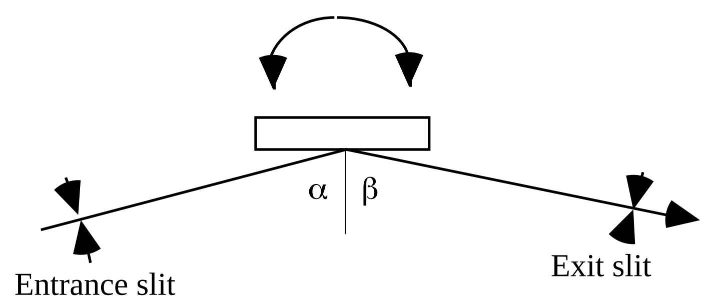
$$\lambda_H = 2d\cos^2\theta$$

- **CONSTANT VALUE OF c_{ff} (SX700)**

$$c_{ff} = \frac{\cos\beta}{\cos\alpha}$$

$$\left(\frac{m\lambda}{d} - \sin\beta\right)^2 = 1 - \left(1 - \sin^2\beta\right)/c_{ff}$$



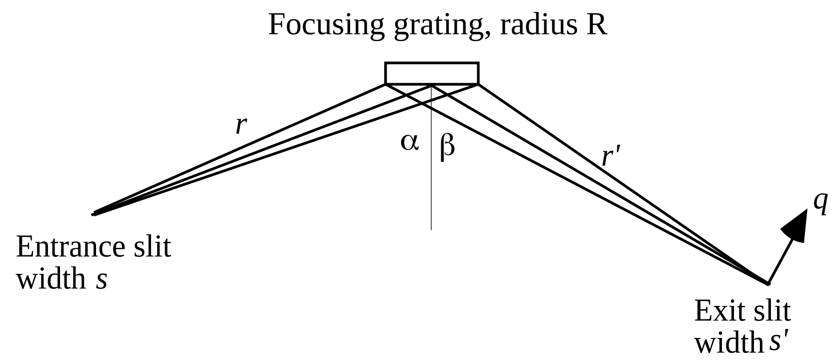


RESOLUTION OF A GRATING SYSTEM

$$m\lambda = d(\sin\alpha + \sin\beta)$$

$$\left(\frac{\partial\lambda}{\partial\beta}\right)_\alpha = \frac{d\cos\beta}{m}$$

$$\frac{d\lambda}{dq} = \frac{d\lambda}{d\beta}\frac{d\beta}{dq} = \frac{d\cos\beta}{mr'} \equiv \frac{10^{-3}d(\text{Å})\cos\beta}{mr'(\text{m})}\ \text{Å}/\text{mm}$$



From this we get the exit- and entrance-slit-width-limited resolutions

$$\boxed{\Delta\lambda_s = \frac{d\cos\alpha\, s}{mr} \qquad \Delta\lambda_{s'} = \frac{d\cos\beta\, s'}{mr'}}$$

Taking the derivative of the grating equation at constant λ. gives the magnification $M(\lambda)$

$$0 = d(\cos\alpha\, d\alpha + \cos\beta\, d\beta)$$

$$M(\lambda) = \frac{s'}{s} = \frac{r'd\beta}{r\,d\alpha} = -\frac{r'\cos\alpha}{r\cos\beta}$$

If $r = R\cos\alpha,\ \ r' = R\cos\beta$ (Rowland circle) $\rightarrow\ M(\lambda) \equiv -1$

Diffraction-limited resolution=1/N

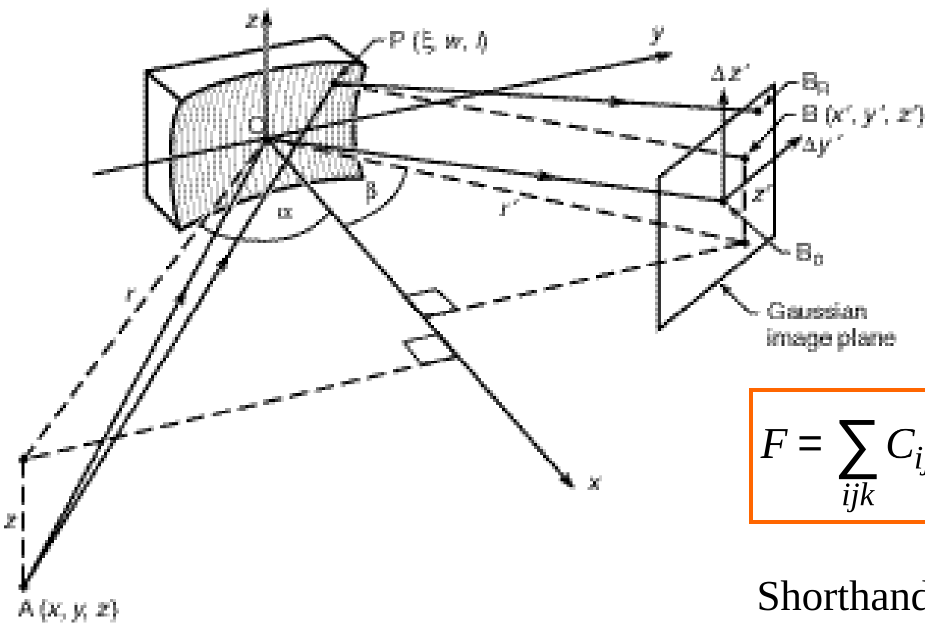
BUT

Provided the grating is big enough, the number of illuminated grooves is always sufficient to achieve the slit-width-limited resolution because of diffraction at the entrance slit

GRATING THEORY

Noda et al 1974

Padmore, Howells & McKinney 2000



OPTICAL PATH FUNCTION THEORY FOR A ROWLAND GRATING

$$F = \langle \mathrm{AP} \rangle + \langle \mathrm{PB} \rangle + mn\lambda = \langle \mathrm{AP} \rangle + \langle \mathrm{PB} \rangle + \frac{m\lambda}{d_0} w$$

where P lies on the surface $\xi = \sum_{ij} a_{ij} w^i l^j$

Now apply standard geometry

$$\boxed{F = \sum_{ijk} C_{ijk}(\alpha, r) w^i l^j z^k + \sum_{ijk} C_{ijk}(\beta, r') w^i l^j z'^k + \frac{m\lambda}{d_0} w}$$

Shorthand notation:

$$T = \frac{\cos^2\alpha}{r} - 2a_{20}\cos\alpha, \qquad S = \frac{1}{r} - 2a_{02}\cos\alpha,$$

$$T' = \frac{\cos^2\beta}{r'} - 2a_{20}\cos\beta, \qquad S' = \frac{1}{r'} - 2a_{02}\cos\beta$$

ABERRATION NAMES

$C_{000} = r$	Constant term
$C_{100} = -\sin\alpha$	Grating equation
$C_{011} = -\dfrac{1}{r}$	Law of reflection in the sagittal plane
$C_{111} = -\dfrac{\sin\alpha}{r^2}$	Line curvature
$C_{102} = \dfrac{\sin\alpha}{r^2}$	Line curvature
$C_{200} = \dfrac{T}{2}$	Tangential-plane defocus
$C_{020} = \dfrac{S}{2}$	Sagittal-plane defocus (astigmatism)
$C_{120} = \dfrac{S\sin\alpha}{2r} - a_{12}\cos\alpha$	Line curvature (also called astigmatic coma)
$C_{300} = \dfrac{T\sin\alpha}{2r} - a_{30}\cos\alpha$	Aperture defect (also called primary coma)
$C_{400} = \dfrac{T\sin^2\alpha}{2r^2} - \dfrac{T^2}{8r} + \dfrac{a_{20}^2}{2r} - \dfrac{a_{30}\sin 2\alpha}{2r} - a_{40}\cos\alpha$	Spherical aberration
$C_{220} = \dfrac{S\sin^2\alpha}{2r^2} - \dfrac{TS}{4r} + \dfrac{a_{20}a_{02}}{r} - \dfrac{a_{12}\sin 2\alpha}{2r} - a_{22}\cos\alpha$	F_{220} aberration

OPTICAL PATH FUNCTION: VARIED-LINE-SPACING GRATINGS

Now the groove spacing *d(w)* and number *n*(w) are functions of w and are also expressed as power series

$$d(w) = d_0\left(1 + v_1 w + v_2 w^2 + \ldots\right) \qquad n(w) = \sum_{i=1}^{\infty} n_{i00} w^i$$

So the optical path function becomes

$$F = \sum_{ijk} C_{ijk}(\alpha, r) w^i l^j z^k + \sum_{ijk} C_{ijk}(\beta, r') w^i l^j z'^k + \frac{m\lambda}{d_0} n_{ijk}$$

$$n_{100} = 1$$

$$n_{200} = -v_1/2$$

$$n_{300} = \left(v_1^2 - v_2\right)/3$$

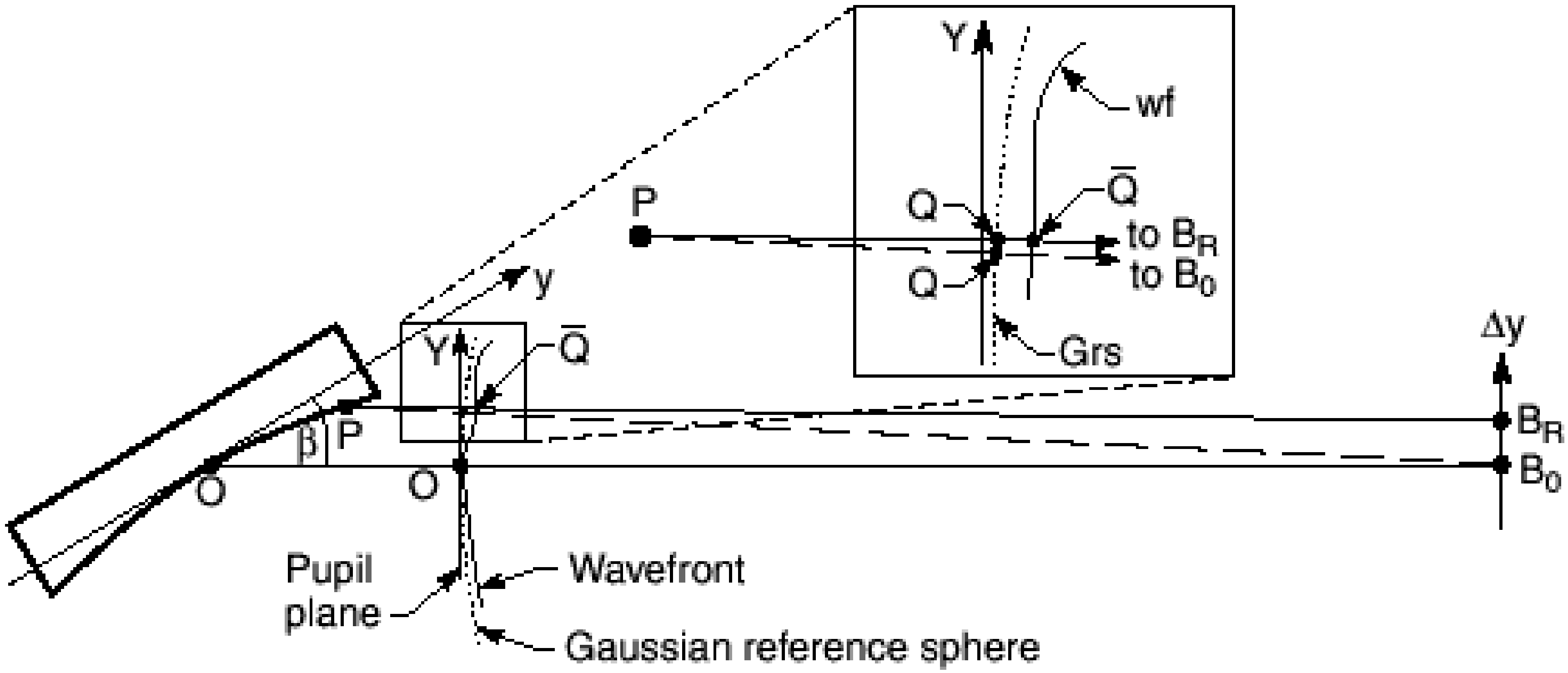
$$n_{400} = \left(-v_1^3 + 2v_1 v_2 - v_3\right)/4$$

$$n_{ijk} = 0 \quad \text{if } i \text{ or } k \neq 0$$

Evidently the use of VLS can benefit aberrations of the form $i00$:

Defocus, coma, spherical aberration but not ones with $j,\ k \neq 0$

THE TRICK YOU NORMALLY DON'T SEE



- We see that the function F is similar to the characteristic function (V) of Hamilton (which would be APB_R in our notation) but is not identical to it because specification of V requires a knowledge of the ray path whereas specification of F does not.
- The approximation needed (which we believe to be true to 8th order) is that $PQ = PQ'$. Using this assumption F can be treated as being equivalent to V.

THE GOAL IS TO KNOW WHERE THE RAYS GO IN THE ABERRATED IMAGE

Padmore, Howells and McKinney (2000) for an explanation

$$\Delta y' = \frac{r_0'}{\cos\beta_0}\frac{\partial F}{\partial w}, \qquad \Delta z' = r_0'\frac{\partial F}{\partial l}$$

Recall that $\Delta y'$ and $\Delta z'$ are the coordinates of the ray arrival point relative to the Gaussian image point. F behaves like a potential and allows them to be calculated. Because F is composed of a sum of terms, we can calculate the contributions of each aberration type separately

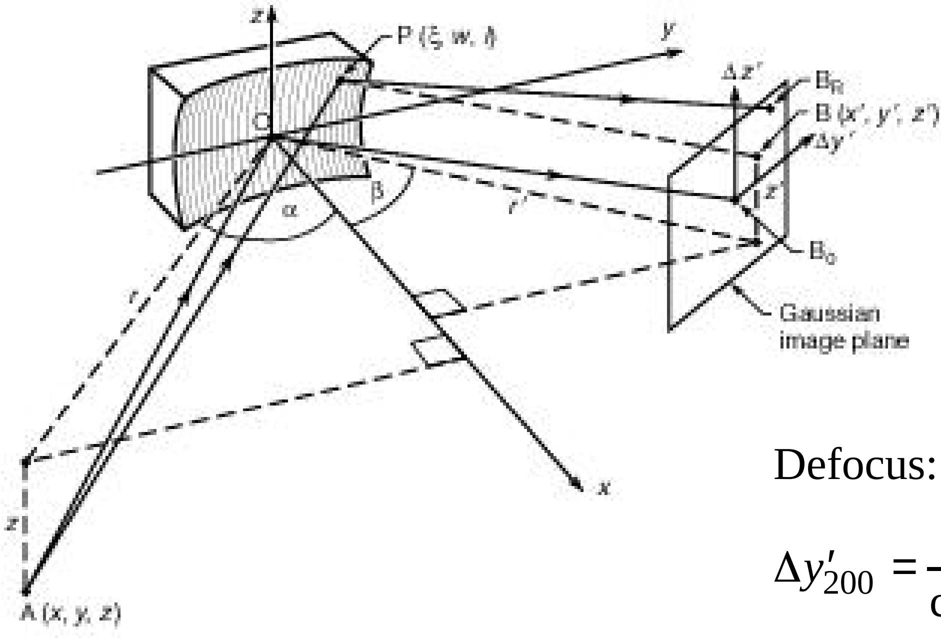
$$\boxed{\Delta y'_{ijk} = \frac{r_0'}{\cos\beta_0}\frac{\partial}{\partial w}\left\{F_{ijk}w^i l^j\right\}, \qquad \Delta z'_{ijk} = r_0'\frac{\partial}{\partial l}\left\{F_{ijk}w^i l^j\right\}}$$

$$\Delta y' = \sum_{ijk}\Delta y'_{ijk}, \qquad \Delta z' = \sum_{ijk}\Delta z'_{ijk}$$

So aberrations can reinforce or cancel each other

Standard practice is to calculate ray positions this way and independently check them against SHADOW ray-traces done with a point source and few rays. When this works and the result looks good, SHADOW can be run with a realistic source and thousands of rays to fully evaluate the design

EXAMPLES OF RAY ABERRATIONS



Defocus:

$$\Delta y'_{200} = \frac{r'_0}{\cos\beta_0}\frac{\partial}{\partial w}\left\{F_{200}w^2\right\} = \frac{r'_0}{\cos\beta_0}\left\{T + T'\right\}$$

Astigmatism:

$$\Delta z'_{020} = r'_0\frac{\partial}{\partial l}\left\{F_{020}l^2\right\} = r'_0\, l\left\{S + S'\right\}$$

Coma

$$\Delta y'_{300} = \frac{r'_0}{\cos\beta_0}\frac{\partial}{\partial w}\left\{F_{300}w^3\right\} = \frac{3}{2}\frac{w^2 r'_0}{\cos\beta_0}\left\{\frac{T\sin\alpha}{r} + \frac{T'\sin\beta}{r'}\right\}$$

- **Generally the focus in the horizontal plane is at a different distance than the focus in the vertical plane**
- **Then the focus consists of two mutually perpendicular focal lines**

CONDITIONS TO BE IN-FOCUS AND COMA-FREE

Spherical grating focus condition:

$$T + T' = \left(\frac{\cos^2\alpha}{r} - \frac{\cos\alpha}{R}\right) + \left(\frac{\cos^2\beta}{r'} - \frac{\cos\alpha}{R}\right) = 0$$

Special cases:

Rowland circle condition: $r = R\cos\alpha$ and $r' = R\cos\beta$

Plane grating case: $R = \infty$

$$r' = -r\frac{\cos^2\beta}{\cos^2\alpha} = -r\,c_{\text{ff}}^2$$

Spherical grating condition for vanishing of coma:

$$\frac{\sin\alpha}{r}\left(\frac{\cos^2\alpha}{r} - \frac{\cos\alpha}{R}\right) + \frac{\sin\beta}{r'}\left(\frac{\cos^2\beta}{r'} - \frac{\cos\alpha}{R}\right) = 0$$

(This condition is satisfied on the Rowland circle)

Applications:

SGM's, TGM's

SGM's

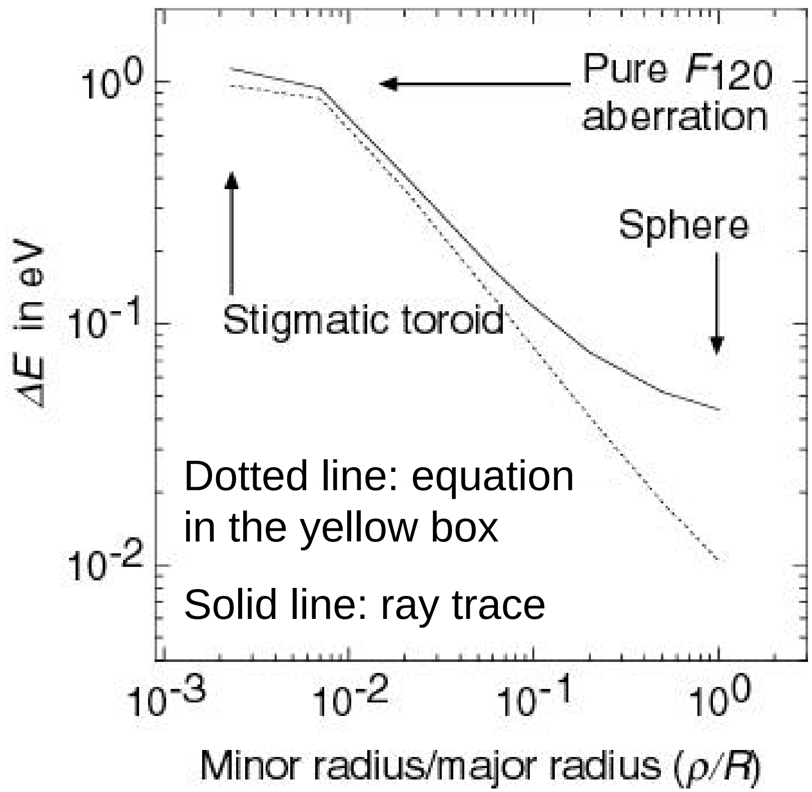
PGM's, SX700 etc

Ultrahigh resolution SGM

CURVATURE OF FOCAL LINES

- **Curved line is represented by** $\Delta y'_{\mathrm{lc}} = k \Delta z'^{2}$
- **The dominant aberration in the *z* direction is normally astigmatism so** $\Delta z'_{020} = r' l \left(S + S' \right)$ **meaning that the length of the focal line is proportional to the ruled length of the grating lines**
- **We need aberration terms that give** $\Delta y'_{\mathrm{lc}} = k \Delta z'^{2}$ **after we have taken the derivative with respect to w and substituted for *l* using the above equation**
- **There are three terms that give this**

$$\Delta y'_{\mathrm{lc}} = \frac{r'_0}{\cos \beta_0} \frac{\partial}{\partial w} \left\{ \frac{1}{2} w l^2 F_{120} + w l F_{111} + w F_{102} \right\}$$



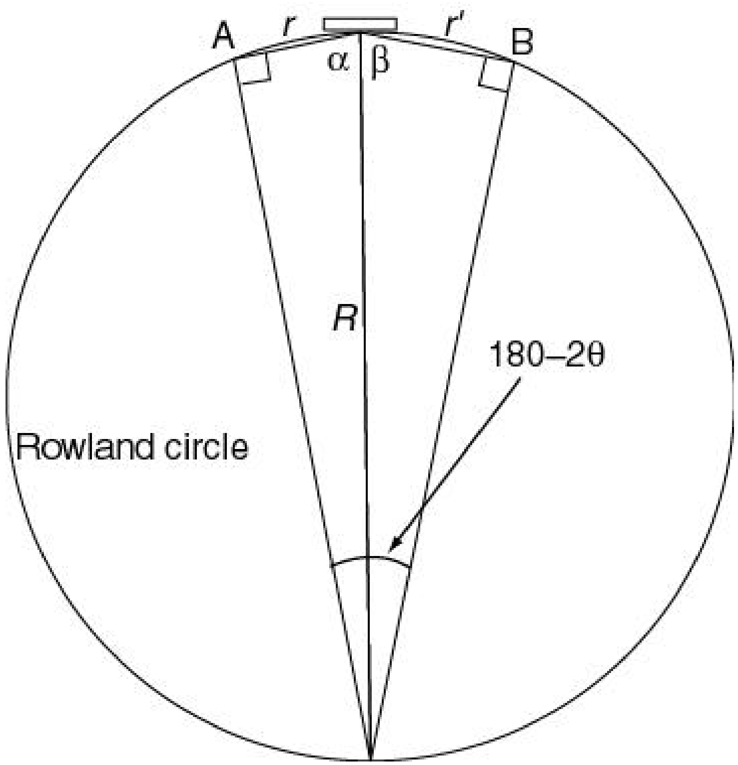
- **Substituting for *l* and the *F*'s we finally get**

$$\boxed{\Delta y'_{lc} = \frac{\Delta z'^{2}}{2 r' \cos\beta \left(S + S' \right)^2} \left[\frac{S \sin\alpha}{r} + \frac{S' \sin\beta}{r'} - \frac{2\left(S + S' \right) \sin\beta}{r'} + \left(S + S' \right)^2 \sin\beta \right]}$$

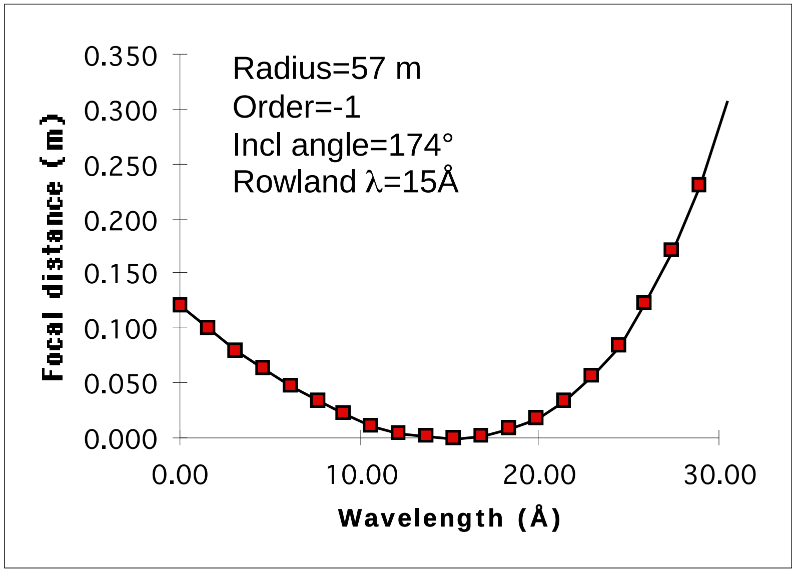
which allows us to calculate *k* and determine the curvature and its contribution to the spectral resolution

THE ROWLAND CIRCLE

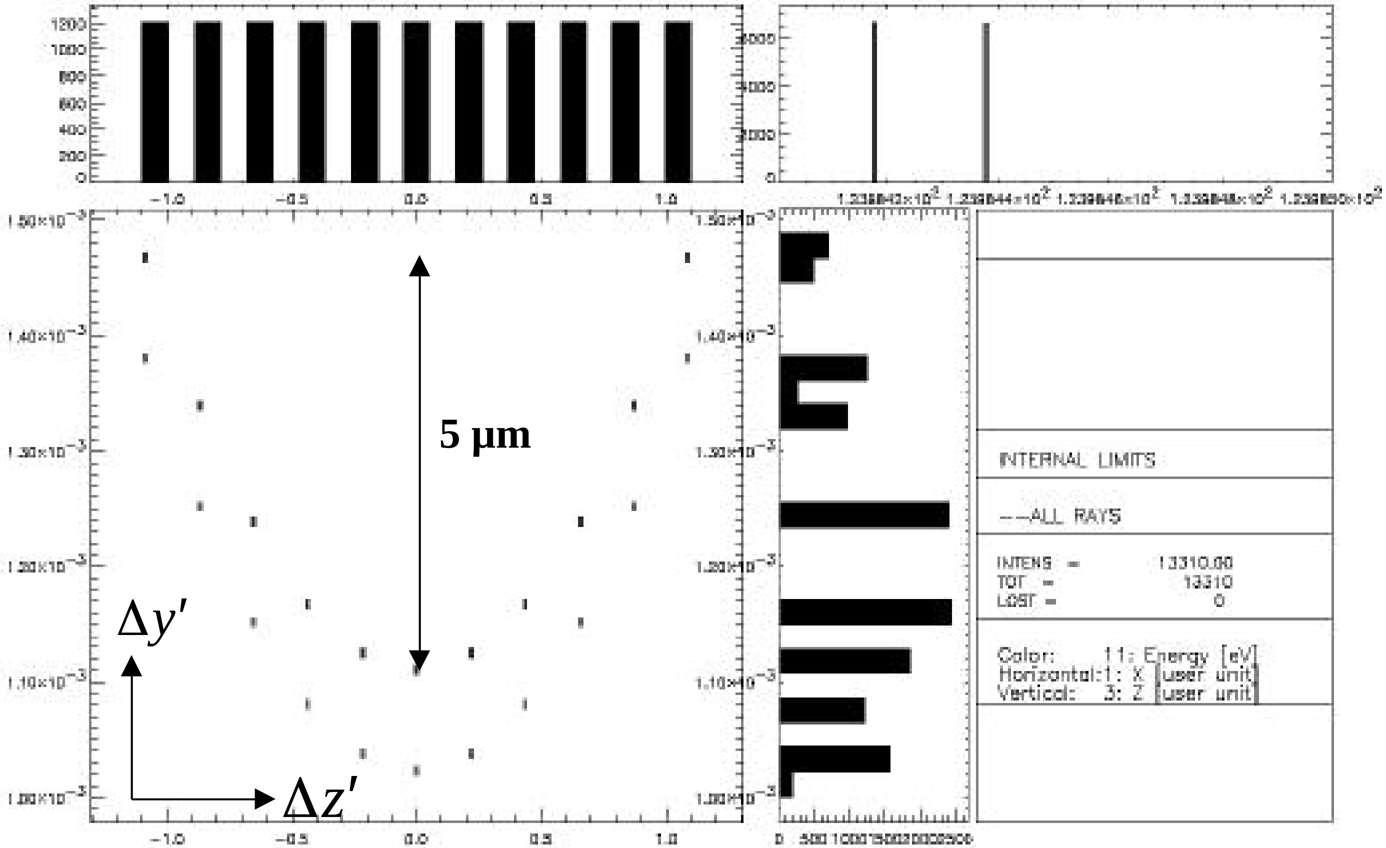
$$r = R\cos\alpha, \;\; r' = R\cos\beta$$



- **Circle of diameter equal to the grating radius**
- **Can choose AB from floor layout considerations and determine *R* from AB=(180–2θ)*R***
- **If the Rowland condition is to satisfied at only one wavelength per grating then it should be below midrange**
- **The Rowland wavelength is a stationary point of the focal distance**



RAY TRACE OF A CANDIDATE SGM DESIGN FOR A "MILLIVOLT RESOLUTION" MONOCHROMATOR



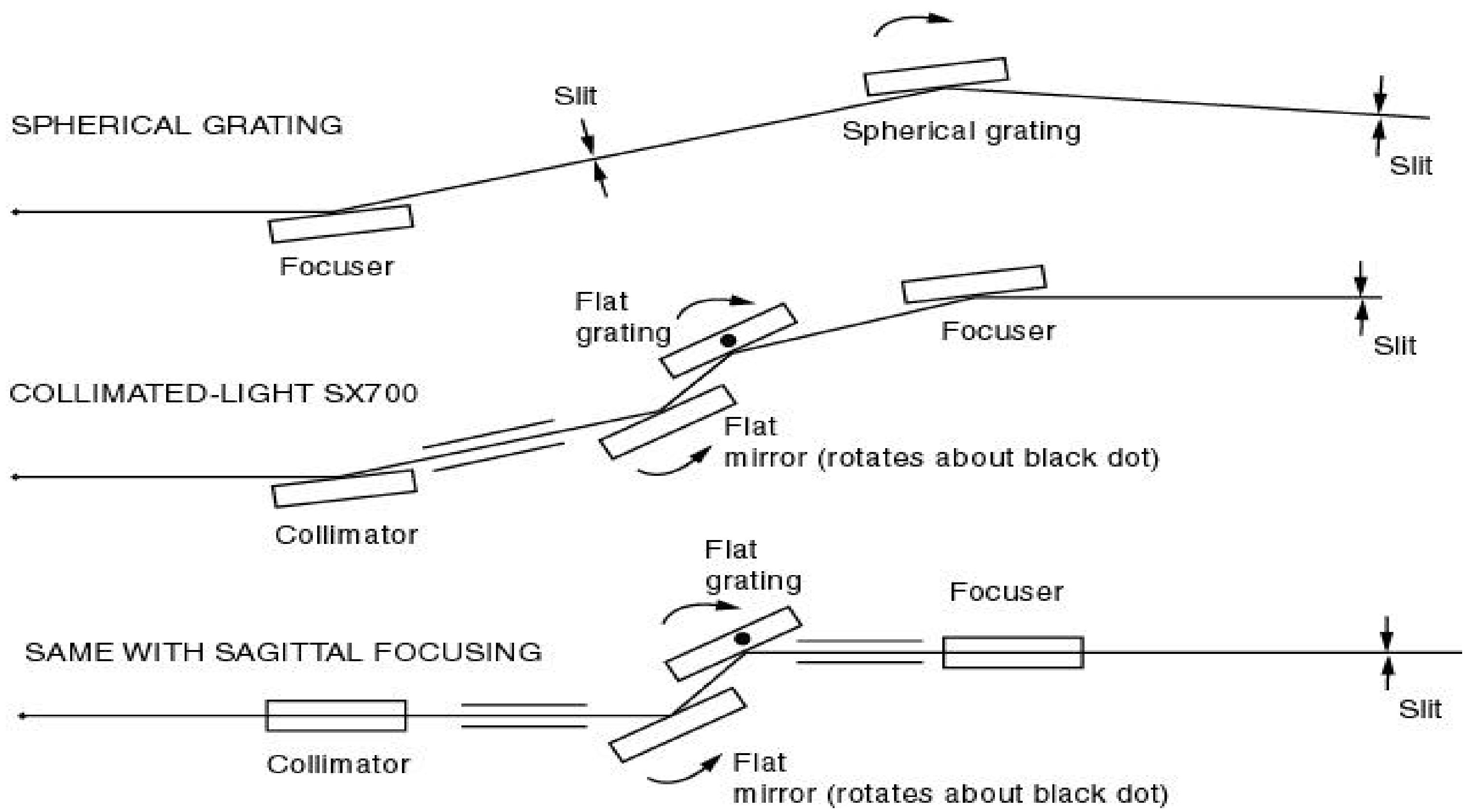
Yi-De Chuang 2002

- **Point source (121 rays)**
- **Fixed angular divergence (from +1.5mrad to −1.5mrad, 0.3 mrad separation) in sagittal plane (X)**
- **Fixed angular divergence (from 0.5 mrad and −0.5 mrad, 0.1 mrad separation) in tangential plane**
- **Two photon energies: 123.98439eV (gray color) and 123.98419eV (black color)**

- **Spherical grating with Roland radius 15.00m**
- **Constant ruling density: 3600 lines/mm**

- Ray trace of two wavelengths 0.2 meV apart
- Note $\Delta y'$ is 4× greater at 4 increments from the center than at 2, i. e. $\Delta y'_{lc} = k\Delta z'^2$ similarly
- The $\Delta z'$ has equally-spaced steps indicating astigmatism
- For a Rowland-circle instrument this is the dominant aberration affecting resolution

CANDIDATE MONOCHROMATOR DESIGNS



ORIGINAL LOGIC OF THE ALS SGM'S

ISSUES THEY SOUGHT TO ADDRESS

- **Optical fabrication tolerances**
- **Optical aberrations (especially of toroidal gratings)**
  - **defocus**
  - **astigmatic coma**
  - **astigmatism**
- **Slit-width limits (especially of low-*R* systems, Grasshopper etc)**
- **Thermal distortions**

Broad concept:
Rense and Viollet 1959

SR monochromators:
Chen 1987
Hogrefe 1986
Padmore 1986

SOLUTIONS THEY OFFERED

- **Optical fabrication tolerances**
  - **Spherical gratings**
  - **SGM's have only one resolution-determining optic (the grating), still significant**
- **Aberrations**
  - **Focus: sliding exit and (perhaps) entrance slits**
  - **Astigmatic coma: spherical (not toroidal) grating**
  - **Primary coma: Rowland circle solution (if entrance slit is moveable)**
  - **Astigmatism: solved by premirror**
- **Slit-width limits**
  - **large radius 10-30 times Grasshopper**
- **Thermal distortion**
  - **internally water-cooled metal gratings**

TODAY'S ASSESSMENT OF THE SGM SOLUTION

- Good response to the challenges of their day but now we see important limitations
- The requirement to move the slit(s) as wavelength is scanned is costly and adversely affects downstream optics somewhat
- The constant deviation angle implies an inability to suppress higher orders by use of the reflectivity
- The tracking of the efficiency maximum on the efficiency-incidence-angle plot is relatively poor especially in the otherwise preferable positive order
- The limited wavelength coverage per grating (about one octave) requires several gratings
- The consequent breaks in the wavelength scan are a serious disadvantage for long-scanning experiments such as SEXAFS
- The ALS SGM's have errors in reproduceability of the wavelength scale when the grating is changed but these can be fixed and are not intrinsic to the SGM design

PRESCRIPTION FOR DESIGNING AN SGM

- Decide the wavelength range and resolution goal and choose 2θ on reflectance grounds for λ_{min}
- Assign the wavelength range so that each grating covers about a factor 2.5 with some overlap between ranges
- Choose the order. This is complicated unless your layout determines which arm must be longer. (m=+1 makes the downstream arm the longer one, m=-1 makes it the shorter one.)
- Consider the shortest wavelength grating only and choose a groove density so that its λ_{max} is about $0.7\lambda_h$ $\left(\lambda_H = 2d\cos^2\theta\right)$
- Consider the center λ of the low λ range and determine its α and β. Determine R from the monochromator length by the Rowland circle geometry and then find the r and r' values that satisfy the focus condition for all wavelengths and thus the amount the slits have to move
- See if it works

SEEING IF IT WORKS

- Calculate the slit-width-limited resolution of the high energy grating for 10 μm slits (about the smallest possible for routine work)
- Calculate the amount of slit movement. Can you build the bellows? Can you afford a slide of the necessary quality? Can the optics of your experiment tolerate this much slit motion?
- Choose a practical (i.e. affordable) size for the grating, usually 10-20 cm. This defines the phase-space acceptance of the system and determines whether it is over or under filled. You need to match the phase-space of the monochromator (at minimum slit setting) to that of the source using the condenser mirror(s). If you cannot avoid overfilling it is better to overfill the slit to reduce the sensitivity to beam movements.
- Calculate the grating surface slope accuracy needed for your resolution goal. Talk to manufacturers and find out what they think you can actually get.
- Calculate the power load (total power and power density) on both the slit and the grating and determine whether you can cool the grating to satisfy the slope tolerance.
- Run your aberration analysis program and get the contribution of each aberration to the resolution broadening. Make an estimate of the overall resolution including the slit sizes, grating manufacturing tolerances and thermally induced slope errors.

WHAT CAN YOU DO IF IT DOESN'T WORK?

This mainly means what if the resolution goal is not achieved?

- Sacrifice wavelength range and use denser gratings. This works even if the problem is slope errors or slit width limits. The trade-off is a smaller λ range per grating and more problems due to breaks in the range
- Use smaller slits. It is hard to build good slits below about 10 µm and the flux goes down like the square of the slit sizes. However, this is what third-generation synchrotron light sources were built for.
- Move the Rowland wavelength around to balance the coma broadening at the top and bottom of the range.
- If coma is still the limit either reduce the illuminated length (w) of the grating (coma diminishes like w^2) or move both slits so as to *always* satisfy Rowland and thereby make the coma vanish exactly. This will probably imply an adaptive-radius condenser mirror.
- Line curvature is normally small but a square-law reduction can be achieved by reducing l. Similarly a cube-law reduction of spherical aberration is achieved by reducing w.
- If the slit motion becomes too great use (i) VLS or (ii) adaptive-radius grating
- If fabrication tolerances are the limit - more money on optics and metrology

WAVELENGTH RANGE OF A CONSTANT-INCLUDED-ANGLE MONOCHROMATOR

- **MINIMUM WAVELENGTH: determined by reflectance**
- **MAXIMUM WAVELENGTH: 60-80% of the horizon wavelength**
- **MULTIPLE GRATINGS:**
  - **- wavelength only appears in the theory as** $m\lambda/d$
  - **- usually within the limit of slit travel we have for each grating** $\lambda_{max} \approx 2.5\lambda_{min}$
- If d and λ are multiplied by n:

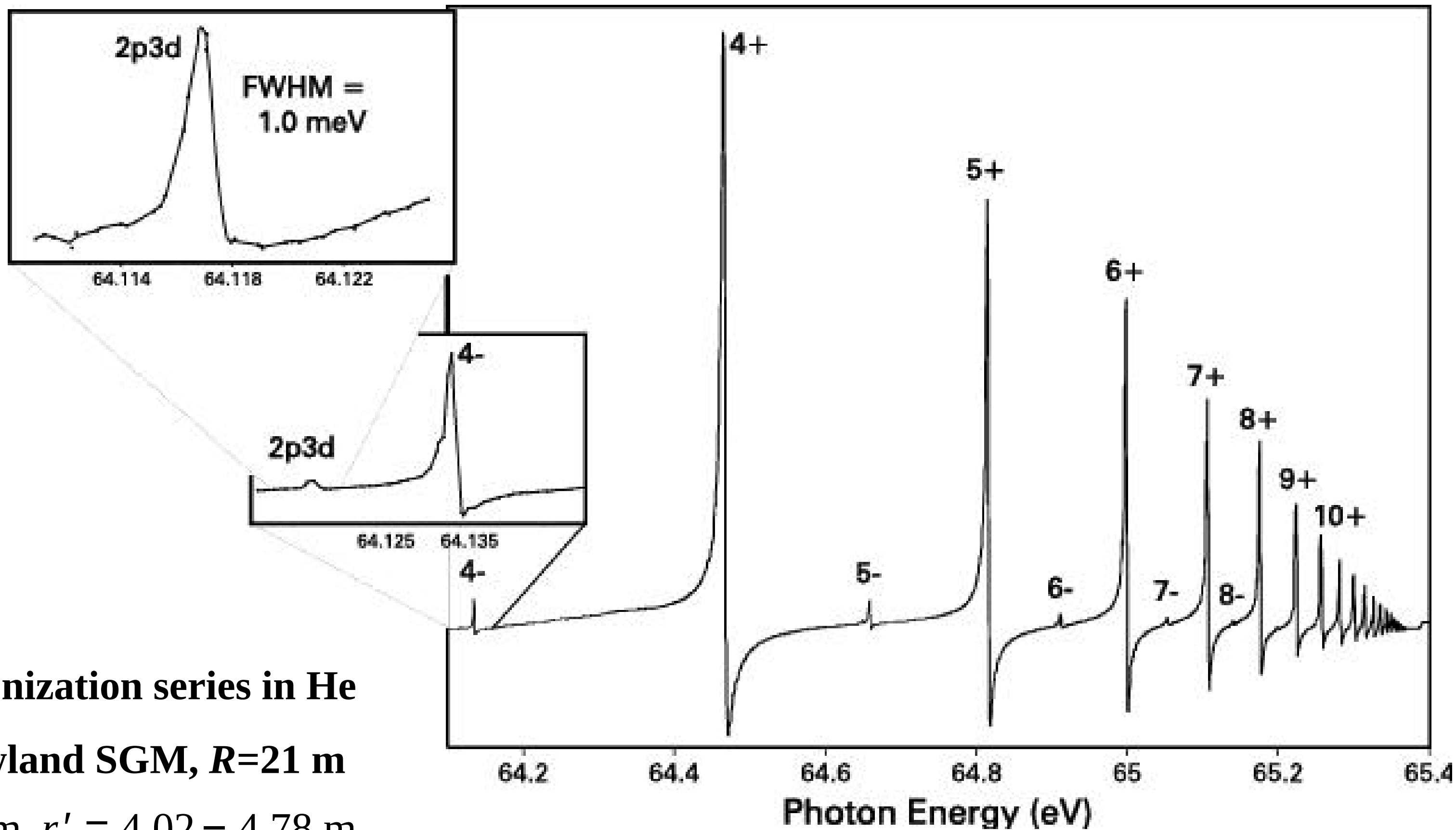
$$\Delta\lambda_{s2} = \frac{s_2 d \cos\beta}{mr'} \quad \rightarrow \quad \Delta\lambda \text{ is } n \text{ times larger}$$

$$E = h\nu = \frac{hc}{\lambda}$$

$$\Delta E = \frac{hc\ \Delta\lambda}{\lambda^2} \quad \rightarrow \quad \Delta E \text{ is } n \text{ times smaller}$$

Resolving power is unchanged

1 meV RESOLUTION BY AN ALS SGM

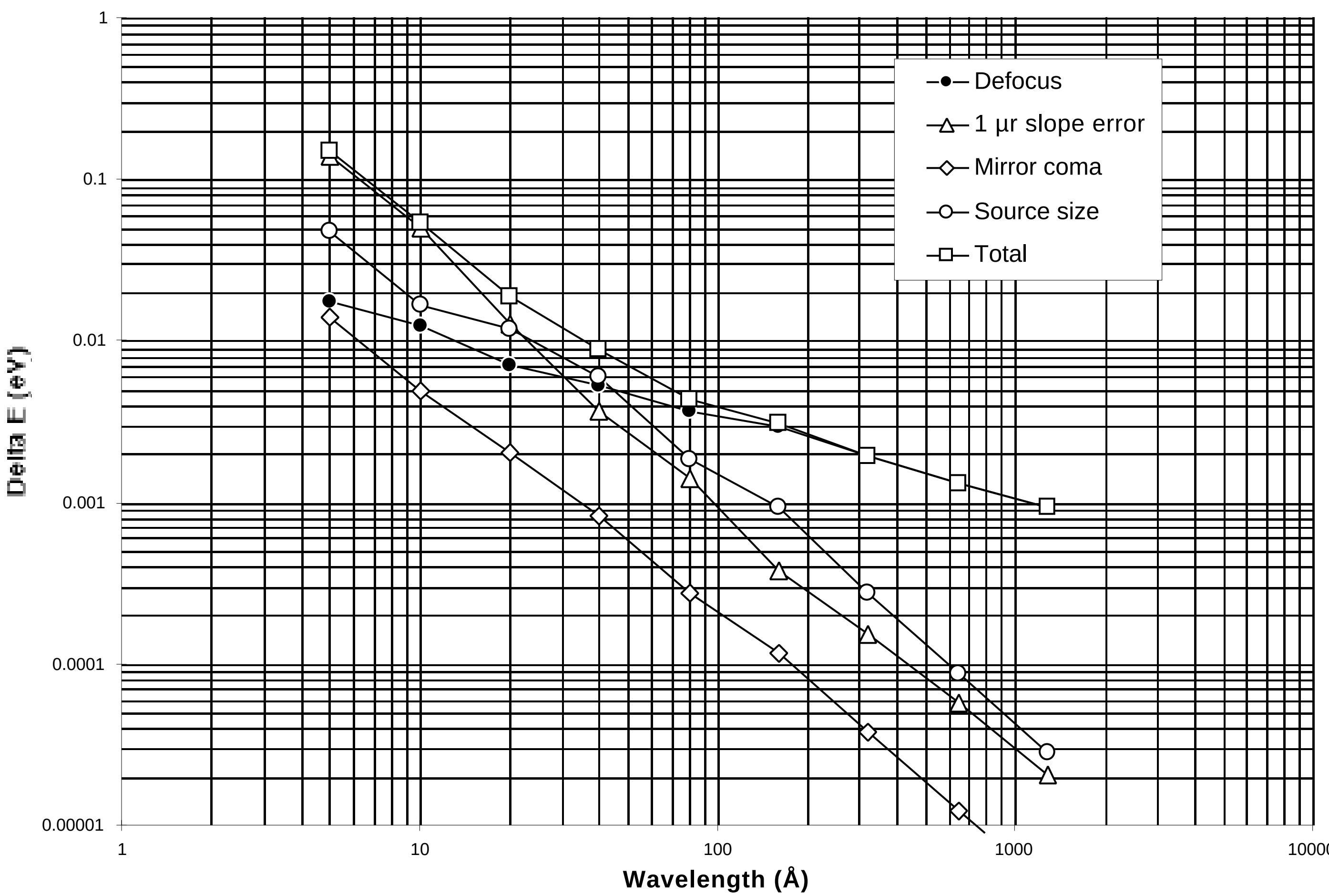


- **Double-ionization series in He**
- **Near Rowland SGM, *R*=21 m**
- $r = 1.45$ m $r' = 4.02 - 4.78$ m
- **1/*d*=925/mm, 2θ=165°m=+1**
- **Closeness to the Rowland wavelength was critical**

ARE SGM'S A CANDIDATE FOR ULTRA HIGH RESOLUTION?

- **The fact that suppression of primary coma is achieved only when the Rowland condition is satisfied implies (a) moving entrance *and* exit slits and (b) adaptive focusing of the condensor mirror. This makes an ultrahigh resolution SGM's costly but alternative solutions have no exact coma supression of at all. Thus SGM's are still in the ultrahigh resolution game although they are now less attractive for a general-purpose beam line**
- **A 100,000-resolving-power SGM at 100Å is not a huge step from what we have already - factor 2 in resolution plus a factor 2 in wavelength**
- **All the subsystems are things where we already have good designs or at least have built them before**
- **SGM's have only one resolution determining optic - the grating - VERY IMPORTANT**
- **Stray light is not cumulative (important for high-density gratings)**
- **There are competitors - the latest PGM's are getting 100,000 resolving power at BESSY - more next week...**

RESOLUTION CONTRIBUTIONS FOR VLS PGM



- Standard SX700
- 600/mm grating
- VLS coefficients
  - v_1=-0.133/m
  - v_2=0.00444/m^2
- Source size=10 μm

SPIE ONE-DAY CLASS

- "Synchrotron Radiation Beam Lines: an Optical engineering Perspective (SC493)"
- Instructor Malcolm Howells
- SPIE Annual Meeting, Seattle 7-11 July 2002
- Class is on Sunday 7th
- Information at http://spie.org
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